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Realistic ghost state: Pauli forbidden state from rigorous solution of the α particle

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The antisymmetrization of the composite particles in cluster model calculations manifests itself in Pauli forbidden states (ghost states), if one restricts oneself to an undeformed cluster in the low-energy region. The resonating group method and the generating coordinate method rely on a property of the norm kernel, which introduces some of the ghost states. The norm kernel has been usually been calculated under the assumption that the inner wave functions have a simple Gaussian form. This is the first time that this assumption has been tested in a rigorous way. In the ${}^4\text{He}+N$ system, we demonstrate a ghost state, which is calculated from a rigorous solution of Yakubovsky equations for the α particle. The ghost states calculated by rigorous and approximate methods turn out to have a very similar form. It is analytically proved that the trace of the norm kernel does not depend on the inner wave function we choose.

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Since 1937 [1], when the resonating group method (RGM) was established, it has been successfully applied to many light nuclei systems. The method is essentially based on the variational principle under the conditions that the clusters remain in the ground state in the low-energy region, and the total wave function is totally antisymmetrized because of the Pauli exclusion principle. A typical example is the two α model [2,3] of ${}^8\text{Be}$. In the 1970's the RGM had great successes [4] and the method was extended to the generating coordinate method (GCM) [5], the orthogonality condition model (OCM) [6], the fish-bone optical model (FBOM) [7], etc. The Pauli exclusion principle plays an important role in the relative motion part of the wave function because it rules out part of the model space by an orthogonality condition. The Pauli forbidden states (ghost states) are generated by diagonalization of an integral kernel in the RGM. The integral kernel is known as the norm kernel (NK) \mathcal{N} which is defined, for example, in the two cluster model as

$$\mathcal{N}(\vec{r}, \vec{r}') \equiv \langle \phi_1 \phi_2 \delta(\vec{r}) | (1 - \mathcal{A}) | \phi_1 \phi_2 \delta(\vec{r}') \rangle, \quad (1)$$

where ϕ_1 , ϕ_2 , and \mathcal{A} are two inner cluster wave functions of the system and an antisymmetrizer for all nucleons, respectively. r is the relative motion coordinate. Namely, the ghost states $u_n(\vec{r})$ are eigenstates of \mathcal{N} with the eigenvalue $\gamma_n = 1$:

$$\int d\vec{r}' \mathcal{N}(\vec{r}, \vec{r}') u_n(\vec{r}') = \gamma_n u_n(\vec{r}). \quad (2)$$

The total wave function Ψ of the system

$$|\Psi\rangle \equiv \mathcal{A} | \phi_1 \phi_2 \chi \rangle \quad (3)$$

is orthogonal to the ghost states $|\phi_1 \phi_2 u_n\rangle$

$$\begin{aligned} \langle \Psi | \phi_1 \phi_2 u_n \rangle &= \langle \phi_1 \phi_2 \chi | \mathcal{A} | \phi_1 \phi_2 u_n \rangle \\ &= \langle \phi_1 \phi_2 \chi | (1 - 1) | \phi_1 \phi_2 u_n \rangle = 0, \end{aligned} \quad (4)$$

where χ is the relative wave function between the two clusters.

Beyond ${}^8\text{Be}$ the α cluster model has been studied in ${}^{12}\text{C}$ [8–10], ${}^{16}\text{O}$ [11], etc. The correct treatment of the Pauli forbidden states is essential even in the case of bound states of clusters, where the neglect of the Pauli principle leads to an extreme overbinding. However, even with the condition they are overbound, which is still a pending problem [12–14] in the α cluster model.

It is analytically proved [15] that if the inner wave functions are simple products of Gaussian functions, then the eigenvectors u_n of Eq. (2) become familiar harmonic oscillator functions. For the sake of simplicity the four spinless cluster (α particle) system in ${}^{16}\text{O}$ has been studied [11] using the Yakubovsky equations [16]. Nowadays, it is possible to obtain rigorous solutions of the α particle wave function using realistic potentials [17]. The recent progress of the $4N$ scattering state is reviewed in Ref. [18]. Therefore, it becomes possible to compare the ghost states which one obtains from the rigorous Yakubovsky solution of the α particle.

In this paper we would like to choose the most simple case, the $\alpha+N$ system. The first four nucleons build up the ground state of the α particle, while the fifth particle is the spectator. The nucleons are identical particles, furthermore, the wave function ϕ_α of α particle is normalized to $\langle \phi_\alpha | \phi_\alpha \rangle = 1$ and NK is defined as Eq. (1),

$$\mathcal{N} = 4 \langle \phi_\alpha \phi_n \delta | P_{45} | \phi_\alpha \phi_n \delta \rangle. \quad (5)$$

P_{45} is the particle exchange operator (4 and 5). Figure 1 suggests the picture of three cluster system ($3N+N+N$). The calculation of the NK is done with Jacobi coordinates which we show in Fig. 2. The relative Jacobi momenta are prepared and the relations between the Jacobi coordinates are

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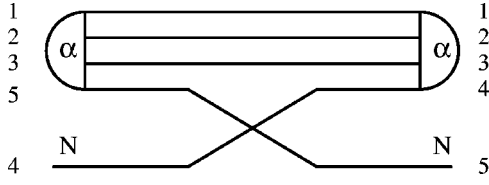


FIG. 1. The diagram of the norm kernel.

$$\vec{p}_1 = \vec{q}_2 + \frac{1}{4}\vec{q}_1, \quad \vec{p}_2 = \vec{q}_1 + \frac{1}{4}\vec{q}_2, \quad (6)$$

where p_i and q_i ($i=1,2$) are Jacobi momenta of $3N+N$ relative motion and $4N+N$ one, respectively.

Our way of calculating the NK is very similar to the calculation of a leading (Born) term of the Alt-Grassberger-Sandhas equations [19,20]. For example, in the text [21] they treat the Born term Z by the partial wave representation with a function $F^{\mathcal{L}}$. In our calculation it is simply replaced as

$$F_{N_1 N_2}^{\mathcal{L}}(q_1, q_2) = \frac{4}{2} \int_{-1}^1 d \cos \theta \left[\int_0^\infty dx \int_0^\infty dy \right. \\ \left. \times \phi_{\alpha; N_1}(x, y, |\vec{p}_1|) \phi_{\alpha; N_2}(x, y, |\vec{p}_2|) \right] P_{\mathcal{L}}(\cos \theta), \quad (7)$$

where the angle θ is between the vectors \vec{q}_1 and \vec{q}_2 , N_1 and N_2 the state channels of the partial wave, and $P_{\mathcal{L}}$ the Legendre function. x and y are rests of Jacobi momenta which describe the motion of particles (1, 2, and 3) inside of the α particle. The numerator 4 is derived from Eq. (5).

As an example, the α wave function [17] of the Argonne potential (AV14) [22] is applied, and we take the case of total spin $J=1/2^+$. For the sake of simplicity we assume the spin j of $3N$ is almost $1/2^+$ (in fact, 94.9% for the case of AV14 potential), therefore, the angular momentum between clusters α and neutron is S wave. This leads to $\mathcal{L}=0$.

Under this choice of the partial waves the recoupling coefficient $A_{N_1, N_2}^{\mathcal{L}}$ [21] is $1/4$ and one gets

$$\mathcal{N}_0(q_1, q_2) = \frac{1}{2} \int_{-1}^1 d \cos \theta \left[\int dx \int dy \right. \\ \left. \times \phi_{\alpha; [1/2^+]}(x, y, p_1) \phi_{\alpha; [1/2^+]}(x, y, p_2) \right] \\ \equiv \frac{1}{2} \int_{-1}^1 d \cos \theta \tilde{\mathcal{N}}(p_1, p_2), \quad (8)$$

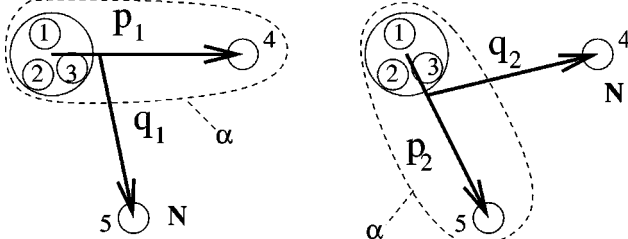
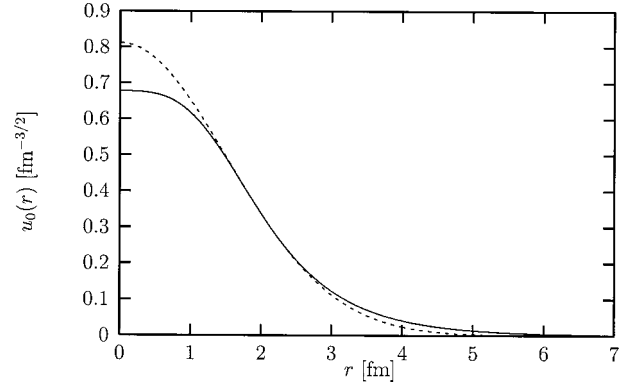


FIG. 2. Jacobi momenta.

FIG. 3. The ghost state in coordinate space. The solid (dashed) line is $u_0^Y(r)$ [$u_0^G(r)$].

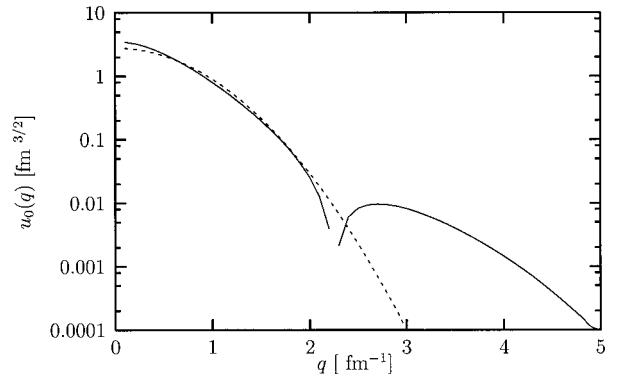
where the subscript “0” of the norm kernel means the angular momentum of \vec{q} and the kernel $\tilde{\mathcal{N}}$ will be used later.

The ghost state is shown in Fig. 3. For our calculation the eigenvalue γ_0 of Eq. (2) is not exactly equal to one, but 0.937 (if it is renormalized by the abovementioned 94.9%, $\gamma_0=0.987$). The solid line is the ghost state u_0^Y calculated from our Yakubovsky solution ϕ_α , comparing to the dashed line from usual Gaussian function

$$u_0^G(r) = \left(\frac{128}{\pi} \omega_{\alpha N}^3 \right)^{1/4} \exp(-\omega_{\alpha N} r^2) \quad (9)$$

with $\omega_{\alpha N} = \Omega \times (4 \times 1) / (4 + 1)$ where Ω is a common shell model mode (0.275 fm^{-2}) [3]. They are normalized by $\int_0^\infty u_n^2(r) r^2 dr = 1$. In the short range our ghost state u_0^Y is smaller than u_0^G . The repulsive core of realistic potentials reflects in this range. This behavior is similar to that of correlation functions [23]. Beyond 4 fm our u_0^Y is bigger than u_0^G because in general the Gaussian function is more quickly decreasing than exponential one. We also show them in the momentum space (see Fig. 4). Here the repulsive core manifests itself by a node at $\approx 2 \text{ fm}^{-1}$ which is absent in u_0^G . Overall they agree well.

To find the most realistic width parameter Ω we optimize $R = |\langle u_0^Y | u_0^G \rangle|^2 \times 100 [\%]$ in Fig. 5. We could recommend $\Omega = 0.24 [\text{fm}^{-2}]$ of the Gaussian width parameter which is similar to $\Omega = 0.275 [\text{fm}^{-2}]$ [3].

FIG. 4. The ghost state ($n=0$) in momentum space. The solid (dashed) line is $u_0^Y(q)$ [$u_0^G(q)$]. The disconnection of the solid line causes from change of sign.

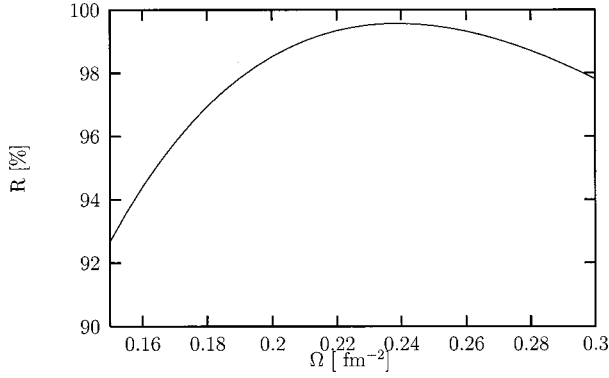


FIG. 5. The percentage R of the ghost state as a function of oscillator parameter Ω .

In Table I we summarize the biggest eigenvalues in Eq. (2). Analytically we find in the Gaussian case eigenvalues $\gamma_n = (-4)^{-(2n+0)}$, $n=0,1,2,\dots$ [15]. The realistic NK has a similar spectrum. We compare the states u_1^Y and u_1^G for $n=1$ in Fig. 6. It is remarkable that in this case the realistic ghost state has more structure though the eigenvalues are very similar.

The matrix traces $\text{Tr}[\mathcal{N}_0]$ are given

$$\text{Tr}[\mathcal{N}_0]^G = \sum_{n=0}^{\infty} \gamma_n = \sum_{n=0}^{\infty} \left(\frac{1}{16}\right)^n = \frac{16}{15} = 1.0666\dots,$$

$$\text{Tr}[\mathcal{N}_0]^Y = \int_0^{\infty} \mathcal{N}_0(q,q) q^2 dq = 1.0125. \quad (10)$$

If the wave function of α particle is renormalized by only $j=1/2^+$, $\int_0^{\infty} p^2 dp \tilde{\mathcal{N}}(p,p) = 1$ (0.949: original norm) we get $\text{Tr}[\mathcal{N}_0]^Y = 1.0666$ which must exactly be the number of the Gaussian form. Because it is analytically proved that the trace $\text{Tr}[\mathcal{N}_0]$ does not depend what kinds of the α wave function we choose

$$\begin{aligned} \text{Tr}[\mathcal{N}_0] &= \int_0^{\infty} \left[\frac{1}{2} \int_{-1}^1 d \cos \theta \right. \\ &\quad \times \tilde{\mathcal{N}} \left(\sqrt{\frac{17}{16} + \frac{\cos \theta}{2}} q, \sqrt{\frac{17}{16} + \frac{\cos \theta}{2}} q \right) \Big] q^2 dq \\ &= \frac{1}{2} \int_{-1}^1 d \cos \theta \frac{1}{\sqrt{17/16 + \cos \theta/2}^3} = \frac{16}{15}. \end{aligned} \quad (11)$$

TABLE I. Eigenvalues of the norm kernel.

n	γ_n	(γ_n^{-1}) of u_n^Y	γ_n	(γ_n^{-1}) of u_n^G [15]
0	0.937	(1.068)	1.00000	(1)
1	0.0663	(15.09)	0.06666	(16)
2	0.00753	(132.0)	0.00391	(256)

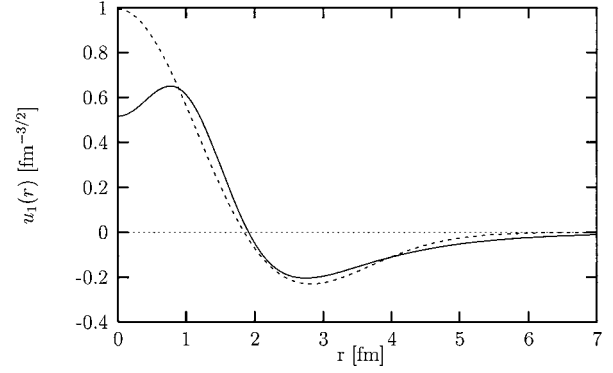


FIG. 6. The eigenstate ($n=1$) of Eq. (2) in coordinate space. The solid (dashed) line is $u_1^Y(r)[u_1^G(r)]$.

We illustrate both NKs (Fig. 7 for \mathcal{N}_0^Y and Fig. 8 for \mathcal{N}_0^G). The Gaussian case is analytically given,

$$\begin{aligned} \mathcal{N}_0(q,q') &= \frac{32}{qq'} \sqrt{\frac{1}{6\pi\Omega}} \\ &\times \exp \left[\frac{17}{48\Omega} (q^2 + q'^2) \right] \sinh \left[\frac{1}{3\Omega} qq' \right]. \end{aligned} \quad (12)$$

The shape is so similar that the difference $(\mathcal{N}_0^Y - \mathcal{N}_0^G)$ is also shown in Fig. 9.

Although there is only a single ghost state in a α - N system, in general, the cluster-cluster effective interaction in light nuclei has a lot of ghost states. In this simple case we could find some remarkable differences in the eigenstate ($n=1$) and the eigenvalue for $n=2$ which might effect RGM calculations of systems with $A>5$. For a most probable case such a Pauli blocking will be applied to the α - n - n three-body model system. There are already some applications [24,25] by using some Pauli methods.

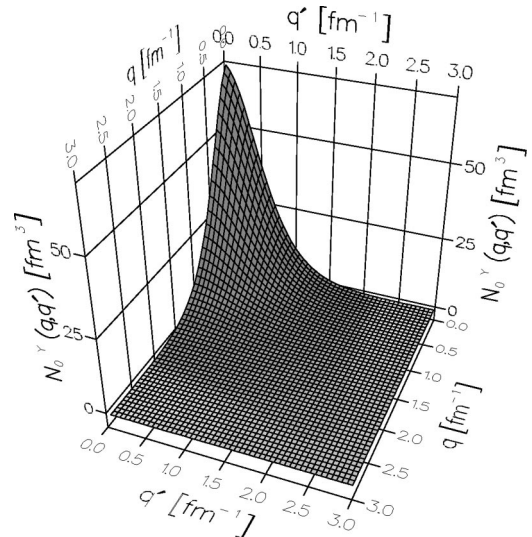
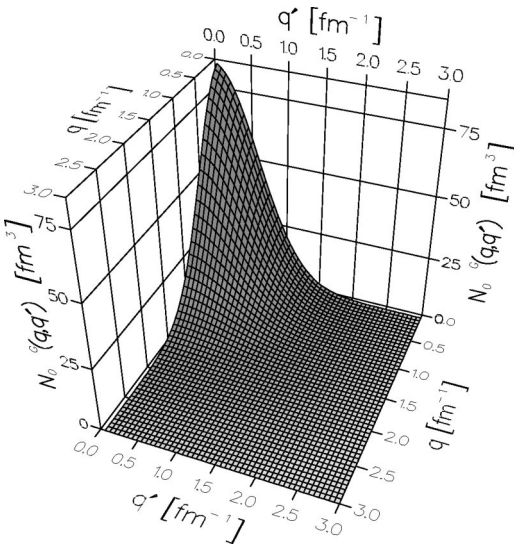
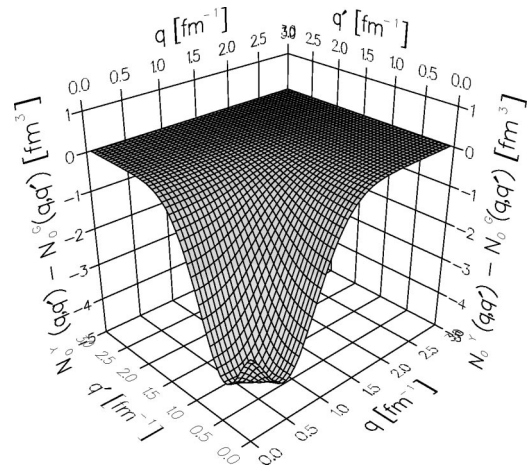


FIG. 7. Norm kernel \mathcal{N}_0^Y .

FIG. 8. Norm kernel \mathcal{N}_0^G .

It will be important for benchmark calculations for systems with more nucleons to look into the ghost states using rigorous solutions [26] from few-body physics. Note that here we discuss the Pauli forbidden state which is different from the spurious state of the Faddeev calculations [27,28]. The term “spurious state” has been used a lot in many places, even if a cluster model has no inner structure the ghost states appear in the model and they are interpreted as kinds of spurious states. We should not confuse spurious

FIG. 9. The difference of the norm kernels ($\mathcal{N}_0^Y - \mathcal{N}_0^G$).

states caused from Faddeev decomposition [27–29]. In this paper we simply take the physical Yakubovsky solution of α particle to test quantitatively how precise the former Gaussian norm kernel is.

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